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6-[(2,4-Dimethylanilino)methylidene]-2-hydroxycyclohexa-2,4-dienone

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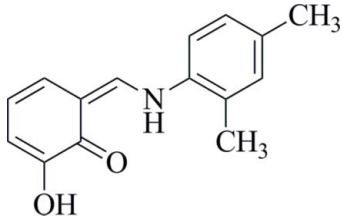
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.043; wR factor = 0.123; data-to-parameter ratio = 10.6.

In the title compound, $C_{15}H_{15}NO_2$, the dihedral angle between the aromatic rings is 5.86 (6)°, and an intramolecular N—H···O hydrogen bond generates an S(6) motif, which helps to stabilize the enamine–keto tautomer. An intramolecular O—H···O hydrogen bond also occurs. In the crystal, inversion dimers linked by pairs of O—H···O hydrogen bonds generate $R_2^2(10)$ loops. A C—H···O interaction links the dimers into [010] chains and aromatic π–π stacking [centroid–centroid separation = 3.6131 (9) Å] also occurs.

Related literature

For a related structure and background to Schiff bases, see: Shuja *et al.* (2007). For further structural aspects, see: Blagus & Kaitner (2011).



Experimental

Crystal data

$C_{15}H_{15}NO_2$
M_r = 241.28
Triclinic, $P\overline{1}$
a = 7.6731 (8) Å
b = 8.4348 (9) Å
c = 10.5806 (12) Å
α = 80.6107 (18)°
β = 75.8216 (19)°
γ = 63.3573 (16)°
V = 592.31 (11) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
0.53 × 0.48 × 0.29 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2006)
T_{min} = 0.943, T_{max} = 0.974
4681 measured reflections
2363 independent reflections
2148 reflections with $I > 2\sigma(I)$
R_{int} = 0.009

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.123
S = 1.09
2363 reflections
223 parameters
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H21···O2	0.85 (2)	2.340 (17)	2.7674 (12)	111.3 (12)
O1—H21···O2^{i}	0.85 (2)	2.00 (2)	2.7320 (13)	143.4 (15)
N1—H31···O2	1.00 (2)	1.72 (2)	2.5873 (12)	142.7 (18)
C13—H13···O1^{ii}	0.980 (14)	2.557 (14)	3.3069 (14)	133.3 (13)

Symmetry codes: (i) $-x, -y+2, -z+1$; (ii) $x, y-1, z$.

Data collection: *SMART* (Bruker, 2006); cell refinement: *SAINT-Plus* (Bruker, 2006); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLUTO* (Meetsma, 2006) and *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB7078).

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supplementary materials

Acta Cryst. (2013). E**69**, o871 [doi:10.1107/S1600536813012233]

6-[(2,4-Dimethylanilino)methylidene]-2-hydroxycyclohexa-2,4-dienone

Shaukat Shujah, Saqib Ali, Zia-ur-Rehman, M. Nawaz Tahir and Auke Meetsma

Comment

As part of our ongoing studies of Schiff bases (Shuja *et al.* 2007), here we report the synthesis and structure of title compound, (I), (Fig. 1). In the molecular structure of (I) the bond distances C7–O2 [1.298 (13) Å] and C1–N1 [1.311 (14) Å] indicate keto-amino tautomeric form. This is further confirmed by a formation of strong intramolecular hydrogen bond N–H···O [N···O = 2.587 (12) Å] resulting in an S(6) ring. The C8–N1–C1–C2 torsion angle is 179.91 (12). The C1–N1 bond length [1.311 (14) Å] is smaller than the N1–C8 bond length [1.417 (14) Å]. The C1–C2 bond length [1.416 (16) Å] indicate a double-bond character and the short C5–C6 bond distance [1.372 (16) Å] of benzene core suggests the presence of quinoid effect (Blagus *et al.*, 2011). The molecules are connected by π–π interactions and O–H···O hydrogen bonds forming a two dimensional network (Fig. 2)

Experimental

An ethanolic solution (50 ml) of 2,4-dimethylaniline (2.5 mmol, 0.30 g) was added dropwise with constant stirring to a hot ethanolic solution (50 ml) of 2,3-dihydroxybenzaldehyde (2.5 mmol, 0.34 g) in a round bottomed flask equipped with a water condenser. The reaction mixture was kept under reflux for 2 h, cooled and kept at room temperature for 48 h. Red blocks of (I) were obtained on slow evaporation of the solvent.

Computing details

Data collection: *SMART* (Bruker, 2006); cell refinement: *SAINT-Plus* (Bruker, 2006); data reduction: *SAINT-Plus* (Bruker, 2006); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLUTO* (Meetsma, 2006) and *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON* (Spek, 2009).

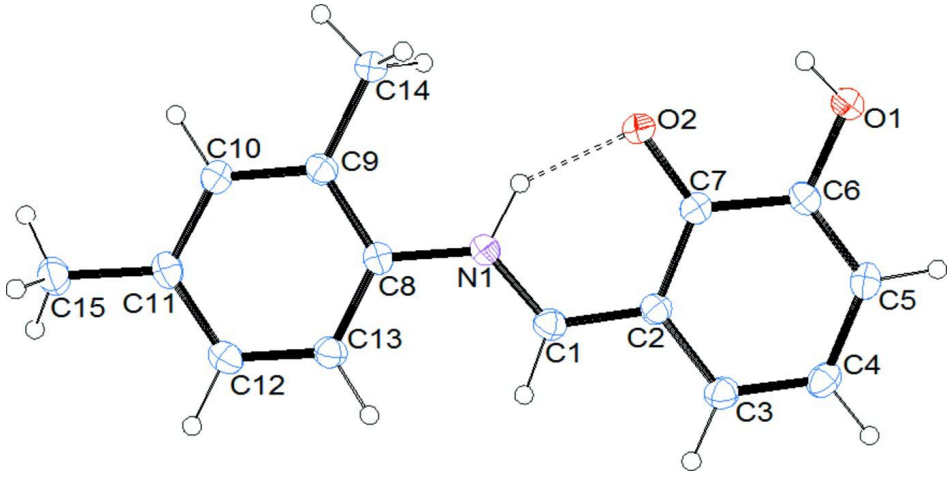

Figure 1

The molecular stucture of (I), with displacement ellipsoids drawn at the 50% probability level. The intramolecular N—H···O hydrogen bond is shown as dashed lines.

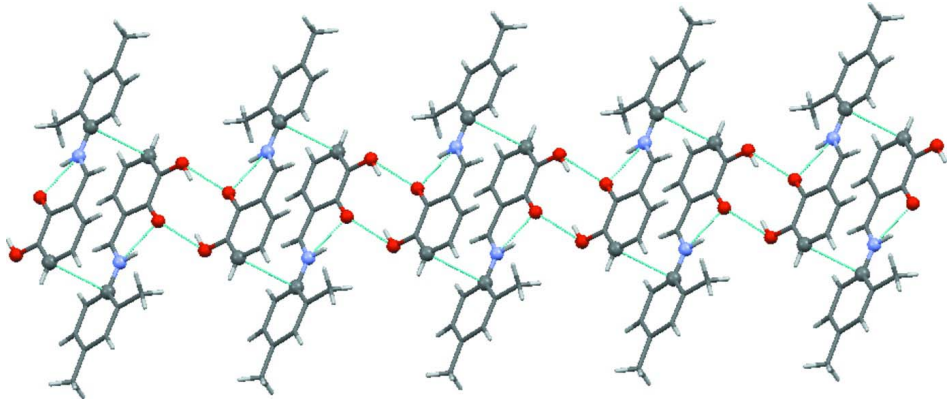

Figure 2

Schiff base molecules connected by π–π interactions and O—H···O hydrogen bonds.

6-[(2,4-Dimethylanilino)methylidene]-2-hydroxycyclohexa-2,4-dienone

Crystal data

$C_{15}H_{15}NO_2$
M_r = 241.28
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 7.6731 (8) Å
b = 8.4348 (9) Å
c = 10.5806 (12) Å
α = 80.6107 (18)°
β = 75.8216 (19)°
γ = 63.3573 (16)°
V = 592.31 (11) Å^3
Z = 2
F(000) = 256

The final unit cell was obtained from the xyz centroids of 3645 reflections after integration using the SAINTPLUS software package (Bruker, 2000).
D_x = 1.353 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3645 reflections
θ = 2.7–29.6°
μ = 0.09 mm^{-1}
T = 100 K
Block, red
0.53 × 0.48 × 0.29 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine focus sealed Siemens Mo tube
Parallel mounted graphite monochromator
Detector resolution: 4096x4096 / 62x62 (binned 512) pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2006)

T_{min} = 0.943, T_{max} = 0.974
4681 measured reflections
2363 independent reflections
2148 reflections with $I > 2\sigma(I)$
R_{int} = 0.009
θ_{max} = 26.4°, θ_{min} = 2.7°
h = −9→9
k = −10→10
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.123
S = 1.09
2363 reflections
223 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: structure-invariant direct methods
Hydrogen site location: inferred from neighbouring sites
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0825P)^2 + 0.0862P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.14548 (13)	0.99696 (10)	0.64979 (8)	0.0261 (3)
O2	0.14914 (11)	0.77675 (9)	0.48083 (7)	0.0213 (2)
N1	0.23552 (13)	0.45820 (12)	0.42735 (8)	0.0179 (3)
C1	0.29515 (15)	0.40370 (14)	0.53911 (10)	0.0198 (3)
C2	0.28631 (15)	0.52113 (14)	0.62454 (10)	0.0180 (3)
C3	0.35444 (16)	0.45246 (14)	0.74426 (10)	0.0214 (3)
C4	0.35457 (16)	0.56226 (14)	0.82597 (10)	0.0217 (3)
C5	0.28454 (16)	0.74722 (14)	0.79198 (10)	0.0209 (3)
C6	0.21286 (16)	0.81822 (14)	0.67902 (10)	0.0195 (3)
C7	0.21212 (15)	0.70814 (14)	0.58908 (10)	0.0178 (3)
C8	0.23908 (15)	0.35066 (13)	0.33599 (10)	0.0173 (3)
C9	0.18384 (15)	0.43224 (13)	0.21664 (10)	0.0182 (3)
C10	0.18940 (16)	0.32622 (14)	0.12556 (10)	0.0194 (3)
C11	0.24356 (16)	0.14426 (14)	0.15117 (10)	0.0203 (3)
C12	0.29389 (16)	0.06799 (14)	0.27204 (11)	0.0215 (3)
C13	0.29397 (16)	0.16855 (14)	0.36332 (10)	0.0201 (3)

C14	0.11771 (17)	0.62921 (14)	0.18686 (10)	0.0220 (3)
C15	0.24119 (18)	0.03446 (15)	0.05288 (12)	0.0250 (3)
H1	0.351 (2)	0.273 (2)	0.5651 (14)	0.034 (4)*
H3	0.400 (2)	0.323 (2)	0.7672 (15)	0.042 (4)*
H4	0.401 (2)	0.5179 (18)	0.9075 (14)	0.027 (3)*
H5	0.286 (2)	0.8279 (19)	0.8468 (14)	0.031 (4)*
H10	0.1540 (19)	0.3814 (17)	0.0398 (13)	0.024 (3)*
H12	0.326 (2)	−0.062 (2)	0.2955 (14)	0.036 (4)*
H13	0.328 (2)	0.1118 (18)	0.4479 (13)	0.026 (3)*
H14	0.218 (2)	0.6672 (19)	0.1967 (14)	0.037 (4)*
H14′	0.096 (2)	0.6606 (19)	0.0969 (14)	0.033 (4)*
H14"	−0.010 (2)	0.6970 (19)	0.2456 (14)	0.033 (4)*
H15	0.251 (3)	0.088 (2)	−0.0373 (18)	0.049 (5)*
H15′	0.353 (2)	−0.084 (2)	0.0470 (16)	0.047 (4)*
H15"	0.122 (3)	0.016 (2)	0.0749 (16)	0.046 (4)*
H21	0.076 (3)	1.025 (2)	0.5909 (19)	0.052 (5)*
H31	0.187 (3)	0.590 (3)	0.412 (2)	0.088 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0360 (5)	0.0169 (4)	0.0268 (4)	−0.0088 (3)	−0.0143 (4)	−0.0005 (3)
O2	0.0259 (4)	0.0177 (4)	0.0188 (4)	−0.0070 (3)	−0.0078 (3)	0.0007 (3)
N1	0.0187 (5)	0.0161 (4)	0.0183 (4)	−0.0068 (3)	−0.0035 (3)	−0.0018 (3)
C1	0.0189 (5)	0.0172 (5)	0.0211 (5)	−0.0060 (4)	−0.0037 (4)	−0.0011 (4)
C2	0.0169 (5)	0.0176 (5)	0.0178 (5)	−0.0058 (4)	−0.0031 (4)	−0.0015 (4)
C3	0.0210 (5)	0.0194 (5)	0.0207 (5)	−0.0057 (4)	−0.0053 (4)	−0.0002 (4)
C4	0.0188 (5)	0.0251 (5)	0.0185 (5)	−0.0061 (4)	−0.0057 (4)	−0.0009 (4)
C5	0.0201 (5)	0.0239 (5)	0.0191 (5)	−0.0086 (4)	−0.0034 (4)	−0.0051 (4)
C6	0.0190 (5)	0.0173 (5)	0.0211 (5)	−0.0069 (4)	−0.0028 (4)	−0.0028 (4)
C7	0.0157 (5)	0.0193 (5)	0.0169 (5)	−0.0066 (4)	−0.0026 (4)	−0.0009 (4)
C8	0.0156 (5)	0.0175 (5)	0.0188 (5)	−0.0070 (4)	−0.0025 (4)	−0.0029 (4)
C9	0.0167 (5)	0.0170 (5)	0.0200 (5)	−0.0067 (4)	−0.0030 (4)	−0.0014 (4)
C10	0.0192 (5)	0.0206 (5)	0.0187 (5)	−0.0083 (4)	−0.0043 (4)	−0.0014 (4)
C11	0.0180 (5)	0.0200 (5)	0.0233 (5)	−0.0081 (4)	−0.0021 (4)	−0.0055 (4)
C12	0.0206 (5)	0.0169 (5)	0.0259 (5)	−0.0073 (4)	−0.0045 (4)	−0.0010 (4)
C13	0.0204 (5)	0.0177 (5)	0.0215 (5)	−0.0074 (4)	−0.0053 (4)	0.0001 (4)
C14	0.0283 (6)	0.0172 (5)	0.0204 (5)	−0.0084 (4)	−0.0083 (4)	0.0002 (4)
C15	0.0275 (6)	0.0221 (5)	0.0272 (6)	−0.0102 (5)	−0.0064 (4)	−0.0061 (4)

Geometric parameters (Å, º)

O1—C6	1.3649 (13)	C10—C11	1.3961 (15)
O2—C7	1.2978 (13)	C11—C12	1.3961 (16)
O1—H21	0.85 (2)	C11—C15	1.5094 (17)
N1—C1	1.3107 (14)	C12—C13	1.3857 (16)
N1—C8	1.4174 (14)	C1—H1	1.005 (15)
N1—H31	1.00 (2)	C3—H3	0.993 (15)
C1—C2	1.4158 (16)	C4—H4	0.968 (15)
C2—C3	1.4237 (15)	C5—H5	0.969 (15)

C2—C7	1.4350 (15)	C10—H10	0.992 (14)
C3—C4	1.3666 (16)	C12—H12	1.012 (15)
C4—C5	1.4184 (15)	C13—H13	0.980 (14)
C5—C6	1.3721 (16)	C14—H14	0.988 (17)
C6—C7	1.4365 (16)	C14—H14′	0.980 (15)
C8—C9	1.4018 (15)	C14—H14"	0.994 (15)
C8—C13	1.3982 (15)	C15—H15	0.987 (18)
C9—C14	1.5061 (15)	C15—H15′	0.982 (16)
C9—C10	1.3989 (15)	C15—H15"	0.96 (2)
O1···O2	2.7674 (12)	C4···H14^{iv}	2.938 (16)
O1···C13^{i}	3.3069 (14)	C4···H14′^{vi}	3.059 (15)
O1···O2^{ii}	2.7320 (13)	C5···H15"^{iii}	2.98 (2)
O1···C14^{ii}	3.3713 (14)	C7···H31	2.35 (2)
O2···O1^{ii}	2.7320 (13)	C12···H3^{vii}	3.096 (15)
O2···C12^{i}	3.4092 (14)	C13···H21^{v}	2.99 (2)
O2···O1	2.7674 (12)	C13···H1	2.635 (15)
O2···N1	2.5873 (12)	C14···H31	2.50 (2)
O2···C13^{iii}	3.2538 (16)	C15···H5^{viii}	2.871 (15)
O1···H13^{i}	2.557 (14)	H1···C13	2.635 (15)
O1···H14"^{ii}	2.633 (14)	H1···H3	2.39 (2)
O2···H31	1.72 (2)	H1···H13	2.07 (2)
O2···H12^{i}	2.649 (16)	H3···H1	2.39 (2)
O2···H21	2.340 (17)	H3···C12^{vii}	3.096 (15)
O2···H21^{ii}	1.999 (19)	H3···H12^{vii}	2.31 (2)
N1···O2	2.5873 (12)	H5···C15^{ix}	2.871 (15)
N1···H14	2.762 (14)	H5···H15^{ix}	2.57 (2)
N1···H14"	2.900 (15)	H5···H15′^{ix}	2.59 (2)
C1···C2^{iv}	3.5296 (18)	H10···C4^{x}	3.015 (14)
C1···C7^{iv}	3.4250 (18)	H10···H14′	2.35 (2)
C2···C9^{iii}	3.4592 (18)	H10···H15	2.46 (2)
C2···C1^{iv}	3.5296 (18)	H10···H10^{xi}	2.55 (2)
C2···C2^{iv}	3.5848 (17)	H12···O2^{v}	2.649 (16)
C4···C9^{iv}	3.4797 (19)	H12···H3^{vii}	2.31 (2)
C4···C8^{iv}	3.4962 (18)	H13···O1^{v}	2.557 (14)
C5···C13^{iv}	3.5694 (19)	H13···C1	2.675 (14)
C5···C8^{iv}	3.3332 (18)	H13···H1	2.07 (2)
C6···C12^{iii}	3.4839 (19)	H13···H21^{v}	2.46 (3)
C6···C11^{iii}	3.4209 (19)	H14···N1	2.762 (14)
C7···C12^{iii}	3.5121 (18)	H14···H31	2.25 (3)
C7···C13^{iii}	3.4649 (19)	H14···C4^{iv}	2.938 (16)
C7···C1^{iv}	3.4250 (18)	H14′···C4^{x}	3.059 (15)
C7···C8^{iii}	3.5955 (18)	H14′···H10	2.35 (2)
C8···C5^{iv}	3.3332 (18)	H14"···N1	2.900 (15)
C8···C4^{iv}	3.4962 (18)	H14"···H31	2.40 (3)
C8···C7^{iii}	3.5955 (18)	H14"···O1^{ii}	2.633 (14)
C9···C2^{iii}	3.4592 (18)	H14"···C1^{iii}	3.048 (16)
C9···C4^{iv}	3.4797 (19)	H15···H5^{viii}	2.57 (2)
C11···C6^{iii}	3.4209 (19)	H15···H10	2.46 (2)

C12···C7^{iii}	3.5121 (18)	H15′···H5^{viii}	2.59 (2)
C12···O2^{v}	3.4092 (14)	H15"···C5^{iii}	2.98 (2)
C12···C6^{iii}	3.4839 (19)	H21···O2	2.340 (17)
C13···C5^{iv}	3.5694 (19)	H21···C13^{i}	2.99 (2)
C13···C7^{iii}	3.4649 (19)	H21···H13^{i}	2.46 (3)
C13···O2^{iii}	3.2538 (16)	H21···O2^{ii}	2.00 (2)
C13···O1^{v}	3.3069 (14)	H31···O2	1.72 (2)
C14···O1^{ii}	3.3713 (14)	H31···C7	2.35 (2)
C1···H14"^{iii}	3.048 (16)	H31···C14	2.50 (2)
C1···H13	2.675 (14)	H31···H14	2.25 (3)
C4···H10^{vi}	3.015 (14)	H31···H14"	2.40 (3)

C6—O1—H21	108.2 (11)	C8—C13—C12	119.90 (10)
C1—N1—C8	126.62 (9)	N1—C1—H1	118.8 (9)
C1—N1—H31	110.9 (13)	C2—C1—H1	118.4 (9)
C8—N1—H31	122.5 (12)	C2—C3—H3	118.1 (9)
N1—C1—C2	122.78 (10)	C4—C3—H3	121.0 (9)
C1—C2—C3	119.73 (10)	C3—C4—H4	122.0 (8)
C1—C2—C7	119.92 (10)	C5—C4—H4	118.2 (8)
C3—C2—C7	120.35 (10)	C4—C5—H5	121.7 (9)
C2—C3—C4	120.82 (10)	C6—C5—H5	117.5 (9)
C3—C4—C5	119.78 (10)	C9—C10—H10	119.3 (8)
C4—C5—C6	120.82 (10)	C11—C10—H10	118.6 (8)
O1—C6—C5	119.25 (10)	C11—C12—H12	119.8 (9)
O1—C6—C7	119.23 (10)	C13—C12—H12	118.9 (9)
C5—C6—C7	121.50 (10)	C8—C13—H13	120.6 (8)
C2—C7—C6	116.70 (10)	C12—C13—H13	119.5 (8)
O2—C7—C2	122.55 (10)	C9—C14—H14	111.6 (8)
O2—C7—C6	120.74 (9)	C9—C14—H14′	109.8 (9)
N1—C8—C13	121.55 (9)	C9—C14—H14"	110.7 (8)
N1—C8—C9	118.11 (9)	H14—C14—H14′	108.3 (13)
C9—C8—C13	120.34 (10)	H14—C14—H14"	108.7 (13)
C8—C9—C10	118.30 (9)	H14′—C14—H14"	107.6 (13)
C8—C9—C14	121.27 (9)	C11—C15—H15	113.3 (11)
C10—C9—C14	120.43 (9)	C11—C15—H15′	113.3 (10)
C9—C10—C11	122.16 (10)	C11—C15—H15"	111.1 (10)
C10—C11—C15	120.97 (10)	H15—C15—H15′	104.2 (14)
C10—C11—C12	118.03 (10)	H15—C15—H15"	107.9 (18)
C12—C11—C15	120.97 (10)	H15′—C15—H15"	106.4 (14)
C11—C12—C13	121.25 (10)		

C8—N1—C1—C2	179.91 (12)	O1—C6—C7—C2	179.47 (11)
C1—N1—C8—C9	−174.84 (12)	C5—C6—C7—O2	−177.99 (12)
C1—N1—C8—C13	5.77 (19)	C5—C6—C7—C2	1.19 (18)
N1—C1—C2—C3	−179.77 (12)	N1—C8—C9—C10	179.26 (11)
N1—C1—C2—C7	−0.87 (19)	N1—C8—C9—C14	−1.44 (18)
C1—C2—C3—C4	177.46 (12)	C13—C8—C9—C10	−1.34 (18)
C7—C2—C3—C4	−1.44 (19)	C13—C8—C9—C14	177.96 (12)
C1—C2—C7—O2	0.84 (19)	N1—C8—C13—C12	179.40 (12)

C1—C2—C7—C6	−178.32 (11)	C9—C8—C13—C12	0.0 (2)
C3—C2—C7—O2	179.74 (12)	C8—C9—C10—C11	1.45 (19)
C3—C2—C7—C6	0.58 (18)	C14—C9—C10—C11	−177.87 (12)
C2—C3—C4—C5	0.53 (19)	C9—C10—C11—C12	−0.20 (19)
C3—C4—C5—C6	1.26 (19)	C9—C10—C11—C15	177.81 (12)
C4—C5—C6—O1	179.58 (12)	C10—C11—C12—C13	−1.2 (2)
C4—C5—C6—C7	−2.1 (2)	C15—C11—C12—C13	−179.20 (12)
O1—C6—C7—O2	0.29 (18)	C11—C12—C13—C8	1.3 (2)

Symmetry codes: (i) *x*, *y*+1, *z*; (ii) −*x*, −*y*+2, −*z*+1; (iii) −*x*, −*y*+1, −*z*+1; (iv) −*x*+1, −*y*+1, −*z*+1; (v) *x*, *y*−1, *z*; (vi) *x*, *y*, *z*+1; (vii) −*x*+1, −*y*, −*z*+1; (viii) *x*, *y*−1, *z*−1; (ix) *x*, *y*+1, *z*+1; (x) *x*, *y*, *z*−1; (xi) −*x*, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H21···O2	0.85 (2)	2.340 (17)	2.7674 (12)	111.3 (12)
O1—H21···O2^{ii}	0.85 (2)	2.00 (2)	2.7320 (13)	143.4 (15)
N1—H31···O2	1.00 (2)	1.72 (2)	2.5873 (12)	142.7 (18)
C13—H13···O1^{v}	0.980 (14)	2.557 (14)	3.3069 (14)	133.3 (13)

Symmetry codes: (ii) −*x*, −*y*+2, −*z*+1; (v) *x*, *y*−1, *z*.